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EXCITATION OF THE HYDROGEN ATOM BY ELECTRON COLLISION

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SUMMARY

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Within the Born approximation and employing parabolic coordinates an expression is found which gives the cross section, induced by electron collision, for excitation of the hydrogen atom from any initial state to any final state. Using this expression the cross section in the energy range of interest in plasma calculations for the following transitions among the principal quantum numbers are tabulated: $n = 1$, $n' = 2, 3, 4, 5, 6, 7, 8, 9, 10$; $n = 2$, $n' = 3, 4, 5, 6, 7, 8$; $n = 3$, $n' = 4, 5, 6, 7, 8$; $n = 4$, $n' = 5, 6$; $n = 5$, $n' = 6$. In conclusion a curve for the total inelastic collision of electrons and the hydrogen atom in its first five energy levels is constructed.

I. INTRODUCTION

The excitation cross section in hydrogen induced by electron collision calculated in the Born approximation is proportional to the squared modulus of the atomic form factor given by

$$V(i, f) = \int e^{iKz} \psi_i(\mathbf{r}) \psi_f^*(\mathbf{r}) d^3\mathbf{r} ,$$

where ψ_i and ψ_f are the initial and final eigenfunctions of the atomic electron and K is the magnitude of momentum transfer of the incident electron. In this paper a closed form is found for the above expression when ψ_i and ψ_f are hydrogenic functions expressed in parabolic coordinates. Elwert[1] (1955) has evaluated this expression with similar specifications, although his final result is in differential form.

The main concern of this paper is the evaluation of the electron impact induced excitation cross section between two arbitrary levels of hydrogen, calculated in the Born approximation. Up to now many calculations in the Born approximation have been carried out in this respect, and tables of cross sections with initial states in the range 1-5 principal quantum numbers and final states 2-10 principal quantum numbers are available,[2-10] although for higher levels the calculations are only for certain substates.

In this paper, after formulation of the problem, the results in parabolic coordinates are compared with those in spherical coordinates, and their consistencies are examined. The calculation is then extended to higher levels, for which results are not available. All cross sections are listed in different tables. It is hoped that these tables will be useful in plasma and astrophysical calculations.

II. FORMULATION

Excitation Amplitude

Let the propagation vector of the exciting electron before and after collision be designated by $\mathbf{k}_0$ and $\mathbf{k}_1$, and the states of the atom in parabolic coordinates before and after collision by $n_1 n_2 m$ and $n_1' n_2' m$. The excitation cross section in atomic units for such a collision is then given by[11]

$$Q(n_1 n_2 m, n_1' n_2' m') = \frac{8\pi}{k_0^2} \int_{k_0-k_1}^{k_0+k_1} \left| V(n_1 n_2 m, n_1' n_2' m) \right|^2 \frac{dK}{K^3}, \tag{1}$$

$$V(n_1 n_2 m, n_1' n_2' m') = \int e^{iKz} \phi_{n_1 n_2 m}(\xi\eta\phi)\, \phi^*_{n_1' n_2' m'}(\xi\eta\phi) \frac{1}{4} (\xi + \eta)\, d\xi\, d\eta\, d\phi$$

$$= \delta(m, m') \frac{1}{4} N_{n_1 n_2} N_{n_1' n_2'} \int_0^\infty \int_0^\infty \exp\left[\frac{iK}{2}(\xi - \eta) - \frac{1}{2}(\alpha + \alpha')(\xi + \eta)\right]$$

$$\times (\xi\eta)^m L^m_{n_1+m}(\alpha\xi)\, L^m_{n_1'+m}(\alpha'\xi)\, L^m_{n_2+m}(\alpha\eta)\, L^m_{n_2'+m}(\alpha'\eta)\, (\xi + \eta)\, d\xi\, d\eta, \tag{2}$$

$N_{n_1 n_2}$ being the normalization factor of the ξ, η eigenfunctions given by Bethe and Salpeter,[12] and also found in I. Similarly, $N_{n_1' n_2'}$ is the factor corresponding to ξ', η'. With this equation and the generating function of the associated Laguerre polynomials (cf. Eq. (37), I) it follows that

$$\sum_{n_1=0}^{\infty}\sum_{n_2=0}^{\infty}\sum_{n_1'=0}^{\infty}\sum_{n_2'=0}^{\infty} \frac{s^{n_1} s'^{n_1'} t^{n_2} t'^{n_2'}}{(n_1+m)!(n_1'+m)!(n_2+m)!(n_2'+m)!} V(n_1 n_2 m, n_1' n_2' m)$$

$$= \frac{\frac{1}{4} N_{n_1 n_2} N_{n_1' n_2'}}{\left[(1-s)(1-t)(1-s')(1-t')\right]^{m+1}} \int_0^\infty \int_0^\infty \exp\left[\frac{iK}{2}(\xi-\eta) - \frac{1}{2}(\alpha+\alpha')(\xi+\eta)\right]$$

$$\times \exp\left[-\left(\frac{\alpha s}{1-s} + \frac{\alpha' s'}{1-s'}\right)\xi - \left(\frac{\alpha t}{1-t} + \frac{\alpha' t'}{1-t'}\right)\eta\right] \times (\xi\eta)^m (\xi+\eta)\, d\xi\, d\eta$$

$$= \frac{-\frac{1}{4} N_{n_1 n_2} N_{n_1' n_2'}}{\left[(1-s)(1-t)(1-s')(1-t')\right]^{m+1}} \frac{\partial U}{\partial p}, \tag{3}$$

where we have introduced

$$p = \frac{1}{2}(\alpha+\alpha'), \qquad q = -\frac{iK}{2}, \tag{4}$$

$$U = \int_0^\infty \exp\left[-\left(p+q+\frac{\alpha s}{1-s} + \frac{\alpha' s'}{1-s'}\right)\xi\right] \xi^m\, d\xi$$

$$\times \int_0^\infty \exp\left[-\left(p-q+\frac{\alpha t}{1-t} + \frac{\alpha' t'}{1-t'}\right)\eta\right] \eta^m\, d\eta$$

$$= (m!)^2 \left(p+q+\frac{\alpha s}{1-s} + \frac{\alpha' s'}{1-s'}\right)^{-(m+1)} \left(p-q+\frac{\alpha t}{1-t} + \frac{\alpha' t'}{1-t'}\right)^{-(m+1)}. \tag{5}$$

Before we carry out the differentiation of U with respect to p, we expand U in powers of s, s', t, t'. Consider the expansion

$$y(s, s') = \left(p + q + \frac{\alpha s}{1 - s} + \frac{\alpha' s'}{1 - s'}\right)^{-(m+1)} = \sum_{\ell_1=0}^{\infty} \sum_{\ell_1'=0}^{\infty} (\ell_1! \ell_1'!)^{-1} y^{\ell_1 \ell_1'}(0, 0)\, s^{\ell_1} s'^{\ell_1'}, \tag{6}$$

$y^{\ell_1 \ell_1'}(0, 0)$ representing the ℓ_1th and the ℓ_1'th derivatives of y(s, t) with respect to s and t, evaluated at s = t = 0. To evaluate $y^{\ell_1 \ell_1'}(s, s')$, it is necessary to introduce

$$u = \frac{\alpha s}{1 - s}, \qquad v = \frac{\alpha' s'}{1 - s'}, \tag{7}$$

then

$$y(u, v) = (p + q + u + v)^{-(m+1)} . \tag{8}$$

It is convenient to introduce also

$$g = (1 - s)^{-1}, \qquad h = (1 - s')^{-1} . \tag{9}$$

Then, making note of the relations

$$\frac{du}{ds} = \alpha g^2 , \qquad \frac{dv}{ds'} = \alpha' h^2 ,$$

$$\frac{d}{ds} g^n = n g^{n+1} , \qquad \frac{d}{ds'} h^n = n h^{n+1} ,$$

it follows that

$$y^{10}(s, s') = \alpha g^2 y'(u, v) ,$$

$$y^{20}(s, s') = \alpha^2 g^4 y^2(u, v) + 2\alpha g^3 y'(u, v) ,$$

$$y^{30}(s, s') = \alpha^3 g^6 y^3(u, v) + 6\alpha^2 g^5 y^2(u, v) + 6\alpha g^4 y'(u, v) ,$$

$y^{\nu}(u, v)$ being the ν^{th} derivative of $y(u, v)$ with respect to either u or v. Inspection of the above equation shows that in general we can write

$$y^{\ell 0}(s, s') = \sum_{\nu=1}^{\ell} C(\nu, \ell)\, \alpha^{\nu} g^{\ell+\nu} y^{\nu}(u, v) ,$$

with $C(\nu, \ell)$ some constants. This equation is identical to Eq. (59), I, provided we let $t \to s'$ and $a_2 \to \alpha$ in the latter equation. The dependence of $y^{\ell 0}(s, s')$ on $y^{\nu}(u, v)$ is then similar to the dependence of $y^{\ell}(s, t)$ on $y^{\nu}(u, v)$ in I, and the $C(\nu, \ell)$ satisfies the following recursion formula (cf. Eq. (60), I)

$$C(\nu, \ell + 1) = (\ell + \nu)\, C(\nu, \ell) + C(\nu - 1, \ell) , \tag{10}$$

with the boundary conditions,

$$C(\nu, \ell) = 0 \text{ when } \nu = 0 \text{ or } \nu > \ell_1 , \quad C(0, 0) = C(1, 1) = 1 . \tag{11}$$

A table of values of $C(\nu, \ell)$ is given in I.

Finally, corresponding to Eq. (61), I, or by direct deduction, we get

$$y^{\ell_1 \ell_1'}(s, s') = \sum_{\nu_1=0}^{\ell_1} \sum_{\nu_1'=0}^{\ell_1'} C(\nu_1, \ell_1)\, C(\nu_1', \ell_1')\, \alpha^{\nu_1} \alpha'^{\nu_1'}\, g^{\ell_1+\nu_1} h^{\ell_1'+\nu_1'}\, y^{\nu_1+\nu_1'}(u, v) \,. \tag{12}$$

Evaluation of $y^{\nu_1+\nu_1'}(u, v)$ when $s = s' = 0$ and substitution of Eq. (12) in Eq. (6) gives

$$\left(p + q + \frac{\alpha s}{1-s} + \frac{\alpha' s'}{1-s'}\right)^{-(m+1)} = \sum_{\ell_1 \ell_1' \nu_1 \nu_1'} (\ell_1 !\, \ell_1' !)^{-1} (-)^{\nu_1+\nu_1'} \times \frac{(m + \nu_1 + \nu_1')!}{m!}$$

$$\times\, C(\nu_1\, \ell_1)\, C(\nu_1'\, \ell_1')\, \alpha^{\nu_1} \alpha'^{\nu_1'} \times a^{-(m+1+\nu_1+\nu_1')} \times s^{\ell_1} s'^{\ell_1'} \,, \tag{13}$$

where we have introduced

$$a = p + q \,. \tag{14}$$

Similarly,

$$\left(p - q + \frac{\alpha t}{1-t} + \frac{\alpha' t'}{1-t'}\right)^{-(m+1)} = \sum_{\ell_2 \ell_2' \nu_2 \nu_2'} (\ell_2 !\, \ell_2' !)^{-1} (-)^{\nu_2+\nu_2'} \times \frac{(m + \nu_2 + \nu_2')!}{m!}$$

$$\times\, C(\nu_2\, \ell_2)\, C(\nu_2'\, \ell_2')\, \alpha^{\nu_2} \alpha'^{\nu_2'}\, a^{*\,-(m+1+\nu_1+\nu_1')}\, t^{\ell_2} t'^{\ell_2'} \,. \tag{15}$$

With substitution of Eqs. (13, 15) in Eq. (5) we find

$$\frac{\partial U}{\partial p} = \left(\frac{\partial}{\partial a} + \frac{\partial}{\partial a^*}\right) U$$

$$= - \sum_{\ell_1 \ell_1' \nu_1 \nu_1' \ell_2 \ell_2' \nu_2 \nu_2'} \left(\ell_1 ! \, \ell_1' ! \, \ell_2 ! \, \ell_2' !\right)^{-1} (-)^{\nu_1+\nu_1'+\nu_2+\nu_2'} \times \left(m + \nu_1 + \nu_1'\right) ! \, \left(m + \nu_2 + \nu_2'\right)!$$

$$\times C\left(\nu_1 \ell_1\right) C\left(\nu_1' \ell_1'\right) C\left(\nu_2 \ell_2\right) C\left(\nu_2' \ell_2'\right) \alpha^{\nu_1+\nu_2} \alpha'^{\nu_1'+\nu_2'}$$

$$\times a^{-(m+2+\nu_1+\nu_1')} a^{*-(m+2+\nu_2+\nu_2')} \times \left[\left(m + 1 + \nu_1 + \nu_1'\right) a^* + \left(m + 1 + \nu_2 + \nu_2'\right) a\right] s^{\ell_1} s'^{\ell_1} t^{\ell_2} t'^{\ell_2'} \tag{16}$$

The right-hand side of Eq. (3) becomes now, after making a binomial expansion of the denominator,

$$\frac{1}{4} N_{n_1 n_2} N_{n_1' n_2'} \sum_{j_1 j_1' j_2 j_2'} \sum_{\ell_1 \ell_1' \nu_1 \nu_1' \ell_2 \ell_2' \nu_2 \nu_2'} \binom{m + j_1}{j_1} \binom{m + j_1'}{j_1'} \binom{m + j_2}{j_2} \binom{m + j_2'}{j_2'}$$

$$\times \left(\ell_1 ! \, \ell_1' ! \, \ell_2 ! \, \ell_2' !\right)^{-1} (-)^{\nu_1+\nu_1'+\nu_2+\nu_2'} \times \left(m + \nu_1 + \nu_1'\right) ! \, \left(m + \nu_2 + \nu_2'\right) !$$

$$\times C\left(\nu_1 \ell_1\right) C\left(\nu_1' \ell_1'\right) C\left(\nu_2 \ell_2\right) C\left(\nu_2' \ell_2'\right) \alpha^{\nu_1+\nu_2} \alpha'^{\nu_1'+\nu_2'}$$

$$a^{-(m+2+\nu_1+\nu_1')} a^{*-(m+2+\nu_2+\nu_2')} \times \left[\left(m + 1 + \nu_1 + \nu_1'\right) a^* + \left(m + 1 + \nu_2 + \nu_2'\right) a\right]$$

$$\times s^{j_1+\ell_1} s'^{j_1'+\ell_1'} t^{j_2+\ell_2} t'^{j_2'+\ell_2'}$$

Equating the coefficients of equal powers of s, s', t, t' of this equation and the left-hand side of Eq. (3), and substituting the value (cf. Eq. (20), I)

$$N_{n_1 n_2} = \left(\frac{2}{n}\right)^{1/2} \alpha^{m+3/2} \left[\frac{n_1!\, n_2!}{(n_1+m)!^3\, (n_2+m)!^3}\right]^{1/2} , \quad \alpha = \frac{Z}{n} , \tag{17}$$

we obtain

$$V(n_1\, n_2\, m,\, n_1'\, n_2'\, m) = \frac{Z^{2m+3}}{2} (n n')^{-(m+2)} \times \left[\frac{n_1!\, n_2!\, n_1'!\, n_2'!}{(n_1+m)!\, (n_2+m)!\, (n_1'+m)!\, (n_2'+m)!}\right]^{1/2}$$

$$\times \sum_{\gamma} \binom{m+j_1}{j_1} \binom{m+j_2}{j_2} \binom{m+j_1'}{j_1'} \binom{m+j_2'}{j_2'} \left(\ell_1!\, \ell_2!\, \ell_1'!\, \ell_2'!\right) (-)^{\nu_1+\nu_2+\nu_1'+\nu_2'}$$

$$\times (m+\nu_1+\nu_1')!\, (m+\nu_2+\nu_2')!\, C(\nu_1\, \ell_1)\, C(\nu_2\, \ell_2)\, C(\nu_1'\, \ell_1')\, C(\nu_2'\, \ell_2')$$

$$\times \alpha^{\nu_1+\nu_2}\, \alpha'^{\nu_1'+\nu_2'} \times \alpha^{-(m+2+\nu_1+\nu_1')} \times a^{*-(m+2+\nu_2+\nu_2')} \times \Big[(m+1+\nu_1+\nu_1')\, a^*$$

$$+ (m+1+\nu_2+\nu_2')\, a\Big] . \tag{18}$$

Here γ stands for the set of 12 variable integers,

$$\gamma = (j_1\, j_2\, j_1'\, j_2'\, \ell_1\, \nu_1\, \ell_2\, \nu_2\, \ell_1'\, \nu_1'\, \ell_2'\, \nu_2') , \tag{19}$$

subject to the restrictions

$$\left.\begin{array}{llll} \ell_1 = 0, 1, 2, \cdots, n_1 \; ; & j_1 = n_1 - \ell_1 \; ; & \nu_1 = 0, 1, 2, \cdots, & \ell_1 \; ; \\ \ell_2 = 0, 1, 2, \cdots, n_2 \; ; & j_2 = n_2 - \ell_2 \; ; & \nu_2 = 0, 1, 2, \cdots, & \ell_2 \; ; \\ \ell_1' = 0, 1, 2, \cdots, n_1' \; ; & j_1' = n_1' - \ell_1' \; ; & \nu_1' = 0, 1, 2, \cdots, & \ell_1' \; ; \\ \ell_2' = 0, 1, 2, \cdots, n_2' \; ; & j_2' = n_2' - \ell_2' \; ; & \nu_2' = 0, 1, 2, \cdots, & \ell_2' \; ; \end{array}\right\} \quad (20)$$

in the transition $n_1 n_2 m \rightarrow n_1' n_2' m$. Eq. (18) gives the desired excitation amplitude.

Integration With Respect to K

When Eq. (18) is substituted in Eq. (1), and the integration is carried out numerically with respect to K, the excitation cross section is obtained. In some cases it is advantageous to carry this integration analitically. To do this, we introduce

$$\beta = \alpha + \alpha' \; ; \qquad (21)$$

then by Eqs. (4, 14), $a = \frac{1}{2}(\beta - iK)$. We introduce further:

$$A = \frac{1}{2}(2Z)^{2m+3}(n n')^{-(m+2)} \times \left[\frac{n_1!\, n_2!\, n_1'!\, n_2'!}{(n_1+m)!\,(n_2+m)!\,(n_1'+m)!\,(n_2'+m)!}\right]^{1/2} \qquad (22)$$

$$G(\gamma) = (-2)^{\nu_1+\nu_2+\nu_1'+\nu_2'} \binom{m+j_1}{j_1} \binom{m+j_2}{j_2} \binom{m+j_1'}{j_1'} \binom{m+j_2'}{j_2'}$$

$$\times \left(\ell_1!\,\ell_2!\,\ell_1'!\,\ell_2'!\right)^{-1} \left(m+\nu_1+\nu_1'\right)!\,\left(m+\nu_2+\nu_2'\right)!\,C\left(\nu_1\,\ell_1\right)\,C\left(\nu_2\,\ell_2\right)\,C\left(\nu_1'\,\ell_1'\right)\,C\left(\nu_2'\,\ell_2'\right)$$

$$\times\ \alpha^{\nu_1+\nu_2}\ \alpha'^{\nu_1'+\nu_2'} \quad , \tag{23}$$

$$H(\gamma) = (\beta - ik)^{-(m+2+\nu_1+\nu_1')} \times (\beta + iK)^{-(m+2+\nu_2+\nu_2')}$$

$$\times \left[\left(2m+2+\nu_1+\nu_2+\nu_1'+\nu_2'\right)\beta + i\left(\nu_1+\nu_1'-\nu_2-\nu_2'\right)K\right] \quad . \tag{24}$$

Then by Eqs. (1, 18) the cross section will be given by

$$Q\left(n_1\,n_2\,m,\,n_1'\,n_2'\,m\right) = \frac{8\pi A^2}{k_0^2} \sum_{\gamma_1=1}^{N} \sum_{\gamma_2=1}^{N} G\left(\gamma_1\right)\,G\left(\gamma_2\right)\,I\left(\gamma_1,\gamma_2\right) \quad , \tag{25}$$

$$I\left(\gamma_1,\gamma_2\right) = \int_{K_1}^{K_2} H\left(\gamma_1\right)\,H^*\left(\gamma_2\right)\,\frac{dK}{K^3} \quad , \tag{26}$$

where N is the number of combinations in the set given by Eq. (19).

By writing

$$H(\gamma) = \left(\beta^2 + K^2\right)^{-(m+2+\nu_1+\nu_2+\nu_1'+\nu_2')} \times (\beta + iK)^{\nu_1+\nu_1'} (\beta - iK)^{\nu_2+\nu_2'}$$

$$\times \sum_{t=0}^{1} a(t)\,(iK)^t$$

$$= \left(\beta^2 + K^2\right)^{-(m+2+\nu_1+\nu_2+\nu_1'+\nu_2')} \sum_{p=0}^{\nu_1+\nu_1'} \sum_{q=0}^{\nu_2+\nu_2'} \sum_{t=0}^{1} (-)^q \binom{\nu_1+\nu_1'}{p} \binom{\nu_2+\nu_2'}{q}$$

$$\times \beta^{\nu_1+\nu_2+\nu_1'+\nu_2'-p-q}\, a(t)\,(iK)^{p+q+t} \quad ,$$

where

$$a(0) = \left(2m + 2 + \nu_1 + \nu_2 + \nu_1' + \nu_2'\right) \beta, \qquad a(1) = \nu_1 - \nu_2 + \nu_1' - \nu_2' \quad , \tag{27}$$

we get

$$I\left(\gamma_1, \gamma_2\right) = \sum_{\omega_1} \sum_{\omega_2} (-)^{\sigma_2} (i)^{\sigma_1+\sigma_2} L\left(\gamma_1, \omega_1\right) L\left(\gamma_2, \omega_2\right) \int \frac{K^{\sigma_1+\sigma_2}\, dK}{K^3 \left(\beta^2 + K^2\right)^{2m+4+\lambda_1+\lambda_2}} \,, \tag{28}$$

where

$$L(\gamma, \omega) = (-)^q \binom{\nu_1+\nu_1'}{p} \binom{\nu_2+\nu_2'}{q} \beta^{\lambda-p-q}\, a(t) \quad ,$$

$$\lambda = \nu_1 + \nu_2 + \nu_1' + \nu_2' \; ; \qquad \sigma = p + q + t \; ; \qquad \omega = (p, q, t) \quad , \tag{29}$$

and each summation extends over all possible values of p, q, t.

Noticing that $I(\gamma_2, \gamma_1) = I^*(\gamma_1, \gamma_2)$, we can write

$$Q(n_1 n_2 m, n_1' n_2' m) = \frac{4\pi A^2}{k_0^2} \sum_{\gamma_1=1}^{N} \sum_{\gamma_2=1}^{N} G(\gamma_1)\, G(\gamma_2) \left[I(\gamma_1, \gamma_2) + I^*(\gamma_1, \gamma_2)\right] . \tag{30}$$

By Eq. (28),

$$I(\gamma_1, \gamma_2) + I^*(\gamma_1, \gamma_2) = \frac{1}{2}\sum_{\omega_1}\sum_{\omega_2} \left[(-)^{\sigma_1} + (-)^{\sigma_2}\right] (i)^{\sigma_1+\sigma_2}\, L(\gamma_1, \omega_1)\, L(\gamma_2, \omega_2)$$

$$\times\, J\left(\frac{\sigma_1 + \sigma_2}{2} - 2,\ 2m + 4 + \lambda_1 + \lambda_2,\ \beta^2,\ x_1\, x_2\right) , \tag{31}$$

where we have defined

$$J(m_1, n_1, a_1, x_1\, x_2) = \int_{x_1}^{x_2} x^m (a + x)^{-n}\, dx . \tag{32}$$

Notice that expression (31) is always real.

Symmetry Considerations

It is evident from Eq. (2) that

$$V\left(n_1 n_2 m, n_1' n_2' m \middle| -K\right) = V^*\left(n_1 n_2 m, n_1' n_2' m \middle| K\right) , \tag{33}$$

$$V\left(n_2 n_1 m, n_2' n_1' m \middle| -K\right) = V\left(n_1 n_2 m, n_1' n_2' m \middle| K\right) . \tag{34}$$

It follows that

$$\left|V\left(n_1\, n_2\, m,\, n_1'\, n_2'\, m \middle| -K\right)\right|^2 = \left|V\left(n_2\, n_1\, m,\, n_2'\, n_1'\, m \middle| K\right)\right|^2 = \left|V\left(n_1\, n_2\, m,\, n_1'\, n_2'\, m \middle| K\right)\right|^2 ; \tag{35}$$

and, by Eq. (1),

$$Q\left(n_2\, n_1\, m,\, n_2'\, n_1'\, m\right) = Q\left(n_1\, n_2\, m,\, n_1'\, n_2'\, m\right) . \tag{36}$$

Eqs. (35, 36) are used to test the accuracy of the numerical results.

Multiplicity of States and the Total Cross Section

Since the direction of the z-axis is taken along the momentum transfer vector **K**, the magnetic quantum number does not change in any transition. As $n_1 + n_2 = n - m - 1$, n_1 can take the values 0, 1, 2, . . . , $n - m - 1$; or $n - m$ values. The same is true of n_2 . Then the total number of combinations of n_1 and n_2 for a given n and m is $n - m$. Similarly, the total number of combinations of n_1' and n_2' for a given n' and m' is $n' - m'$.

Designating the cross section for the transition $nn_1 n_2 m \to n'\, n_1'\, n_2'\, m$ by $Q(nn_1 n_2 m, n' n_1' n_2' m)$, the cross section for the transition $nn_1 n_2 m \to n' m$ is obtained by summing the former cross section over all the final states with a fixed m,

$$Q(nn_1 n_2 m, n' m) = \sum_{n_1'=0}^{n'-m-1} Q(nn_1 n_2 m, n' n_1' n_2' m), \tag{37}$$

The cross section for the transition $nm \rightarrow n'm$ is obtained by averaging $Q(nn_1n_2m, n'm)$ over all the initial states with a fixed m,

$$Q(nm, n'm) = (n-m)^{-1} \sum_{n_1=0}^{n-m-1} Q(nn_1n_2m, n'm). \tag{38}$$

The cross section for the transition $n \rightarrow n'$ is obtained by averaging $Q(nm, n'm)$ with respect to the magnitude of the magnetic quantum number m,

$$Q(n, n') = (2n-1)^{-1} \sum_{m=0}^{n-1} \left[2 - \delta(m,o)\right] Q(nm, n'm). \tag{39}$$

Since the total number of the initial states is

$$\sum_{m=0}^{n-1} \left[2 - \delta(m,o)\right] (n-m) = n^2, \tag{40}$$

Eq. (39) can be written alternatively as

$$Q(n, n') = n^{-2} \sum_{m=0}^{n-1} \sum_{n_1=0}^{n-m-1} \left[2 - \delta(m, o)\right] Q(nn_1n_2m, n'm) . \tag{41}$$

It is interesting to note that the number of independent transitions between the levels n and n' is given by

$$N = \sum_{m=0}^{n-1} [2 - \delta(m, o)] (n-m)(n'-m).$$

When the right hand side is evaluated we obtain

$$N = n^2 \left(n' - \frac{n}{3}\right) + \frac{n}{3}. \tag{42}$$

III. RESULTS AND DISCUSSION

We have calculated within the Born approximation the excitation cross section of the hydrogen atom by electron collision for the transitions $n = 1$ to $n' = 2, 3, 4, 5, 6, 7, 8, 9, 10$; $n = 2$ to $n' = 3, 4, 5, 6, 7, 8$; $n = 3$ to $n' = 4, 5, 6, 7, 8$; $n = 4$ to $n' = 5, 6$; and $n = 5$ to $n' = 6$ by employing parabolic coordinates. Previous similar calculations in the Born approximation using spherical coordinates have been made for the transitions $n = 1$ to $n' = 2, 3, 4, 5, 6$ by Mc Carroll[4]; $n\ell = 2s$ to $n' = 3, 4, 5, 6, 7, 8, 9, 10$ by Boyd[5]; $n\ell = 2p$, $m = 0, 1$ to $n' = 3, 4, 5, 6, 7, 8, 9, 10$ by McCrea and McKirgan[6]; $n = 3$ to $n' = 4$ by McCoyd, Milford and Wahl[7]. There are few other calculations for certain optically allowed transitions between sublevels of higher levels but they do not give the total transition cross section between two levels.

As a check on the consistency of the calculations, comparisons are made in this paper with all the values available in spherical coordinates. Table I gives the excitation cross section from the ground state in both coordinates. The agreement is excellent. The cross section due to all higher states which are not listed explicitly can be calculated by a method given in Ref. 4. This is designated by $\sum_{i=n+1}^{\infty} Q(1, i)$, where n is the upper state of the highest transition whose cross section is listed in the table. $Q(T)$ is the total excitation cross section.

Table II compares the cross sections in the two coordinates for the transition $n = 2$ to $n' = 3$. Theoretically we must have

$$Q(2p\pm 1) = Q(00,\ 01) + Q(00,\ 10) = 2Q(00,\ 01) \tag{43}$$

$$\begin{aligned} Q(2s) + Q(2p\,0) &= Q(01,\ 02) + Q(01,\ 11) + Q(01,\ 20) \\ &\quad + Q(10,\ 02) + Q(10,\ 11) + Q(10,\ 20) \\ &= \left[2\ Q(01,\ 02) + Q(01,\ 11) + Q(01,\ 20)\right] \ , \end{aligned} \tag{44}$$

where $Q(n_1 n_2,\ n_1' n_2')$ is the cross section for the transition between the sublevels $n_1 n_2$ and $n_1' n_2'$, and where use has been made of the symmetry relation (36). The above equations are shown to be satisfied in Table II. $Q(2,\ 3)$ is the excitation cross section for the transition $n = 2$ to $n' = 3$, averaged over the initial states and summed over the final states.

For brevity in the remaining of the tables only the averaged cross section for transition between the principal quantum numbers are listed. Table III gives the cross section for the transitions $n = 2$ to $n' = 4, 5, 6, 7, 8$, and the total excitation cross section from the $n = 2$ level. Table IV is constructed to verify the excitation cross sections for $n = 3$ to $n' = 4$ as obtained in Ref. 7. Although the agreement is satisfactory, at low energy the two results differ to some extent. As our values are obtained both by the closed and the integral forms, and in the case of the integral form convergence to the numbers given is achieved by decreasing the mesh sizes of the numerical integration, it is believed that our results are more accurate.

Table V gives the excitation cross section for the $n = 3$ to the $n' = 4, 5, 6, 7, 8$ levels, and the total excitation cross section from the $n = 3$ level. The contribution to the total cross section of the states not listed is obtained by the method outlined in Ref. 4 and the known value of ionization of the $n = 3$ as given in I.

To test the accuracy of the Born approximation, it is necessary to compare the result of the Born calculation with experiment. This is done in Fig. 1 along with the more elaborate theoretical calculation of close coupling [13, 14], and the classical theory of excitation given by Gryzinski [15]. According to this classical theory, if the energy of the incident electron is given as E_0 in rydberg and the atom is excited from the state n to n', the excitation cross section is given by

$$Q(n, n') = \sigma_0 n^4 a(1+a)^{-3/2} \left(\frac{g(n, n')}{\left[1 - \left(\frac{n}{n'}\right)^2\right]^2} - \frac{g(n, n'+1)}{\left[1 - \left(\frac{n}{n'+1}\right)^2\right]^2} \right) ,$$

$$g(n, n') = \begin{cases} -ay^2 + (1+a)y - \frac{1}{3} , & ay \leq 1 , \\ \frac{2}{3}\left[-ay^2 + (1+a)y\right]^{3/2} , & ay \geq 1 , \end{cases}$$

$$\sigma_0 = 4.0307\pi a_0^2 , \qquad a = \left(n^2 E_0\right)^{-1} , \qquad y = 2 - \left(\frac{n}{n'}\right)^2 . \qquad (45)$$

Compared to experiment, the Born approximation gives too high values, the classical theory gives too low, and the close coupling approximation gives the best agreement.

The disagreement between Born calculations and experiment may get worse for the excitation of higher states. This is due to the form of the wave function of the bound electron. Since hydrogenic wave function is used to evaluate the matrix elements of the Born calculations, it is implicitly assumed that the interaction potential between the two electrons is small compared with the interaction of the nucleus and the atomic electron. This, however, may not be the case for the excited states where the average distance of the electron from the nucleus is large.

Fig. 2 compares different excitation cross sections and the ionization cross section of the $n = 1$ level. Figs. 3 and 4 make the same comparison for the $n = 2$ and the $n = 3$ levels.

Table VI gives the excitation cross section of $n = 4$ to $n' = 5, 6$; and the total excitation cross section for this level, while Table VII gives the excitation cross section of $n = 5$ to $n' = 6$. Figs. 5 and 6 show the results of these tables graphically. In Fig. 6 the classical curve is also drawn for comparison. The classical description of the excitation is open to question as transition to discrete levels cannot be described classically.

Although the excitation of the ground state of hydrogen to the 2p state has an order of magnitude larger cross section than the excitation to the 2s state, especially at high incident electron energies[13,14], it should be argued that this does not mean that for the excitation of higher states the cross section of non-optically allowed transitions can be neglected. This neglect is valid when $Ka \ll 1$, where K is the magnitude of the momentum transfer of the incident electron and a is the extent of the charge distribution of the bound electron before and after collision. For the excitation of high levels, a becomes more than an order of magnitude larger than the corresponding a for the ground state. This fact is evidenced by noting that the excitation cross section for optically allowed transitions in $n = 5$ to $n' = 6$ given in Ref. 9 is considerably lower than that given in Fig. 6. Similarly it can be argued that the dipole approximation within the Born approximation becomes less valid for excitation of the higher levels.

Fig. 7 gives the total inelastic cross section by electron collision, including excitations to all levels and ionizations, for the first 5 levels of atomic hydrogen.

In closing it should be mentioned that the cross section for de-excitation induced by electron collision is obtained through

$$Q(f, i) = \frac{k_i}{k_f} Q(i, f) ,$$

where $Q(i, f)$ is the corresponding excitation, and k_i and k_f are the initial and final wave numbers of the incident electron in the excitation process.

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Table I. Excitation cross section of n = 1 level in units of πa_0^2. S is for spherical[a], and P is for parabolic, coordinates used in the calculation of the cross sections.

Impact Energy		Q(1,2)		Q(1,3)		Q(1,4)		Q(1,5)		Q(1,6)		Q(1,7)	Q(1,8)	Q(1,9)	Q(1,10)	$\sum_{i=n+1}^{\infty} Q(1,i)$	Q(T)
ryd	eV	S	P	S	P	S	P	S[b]	P	S[b]	P	P	P	P	P		
1.00	13.60	1.2868	1.2868	0.1787	0.1787	0.0509	0.0509	0.0202	0.0199	0.0092	0.0092	0.0050	0.0032	0.0018	0.0012	0.0016	1.5583
1.44	19.58	1.5354	1.5354	0.2782	0.2782	0.1000	0.1000	0.0476	0.0476	0.0265	0.0265	0.0163	0.0104	0.0075	0.0054	0.0242	2.0515
1.96	26.66	1.4993	1.4993	0.2798	0.2798	0.1021	0.1021	0.0490	0.0490	0.0274	0.0274	0.0169	0.0112	0.0078	0.0056	0.0250	2.0241
2.56	33.43	1.3886	1.3886	0.2600	0.2600	0.0951	0.0951	0.0457	0.0457	0.0256	0.0256	0.0158	0.0104	0.0073	0.0053	0.0234	1.8772
3.24	44.06	1.2630	1.2630	0.2358	0.2358	0.0862	0.0862	0.0413	0.0413	0.0231	0.0232	0.0143	0.0096	0.0066	0.0048	0.0208	1.7056
4.00	54.40	1.1424	1.1424	0.2123	0.2123	0.0775	0.0775	0.0372	0.0372	0.0208	0.0208	0.0128	0.0088	0.0059	0.0043	0.0189	1.5409
6.25	85.00	0.8919	0.8919	0.1637	0.1637	0.0595	0.0595	0.0285	0.0285	0.0159	0.0160	0.0098	0.0064	0.0045	0.0033	0.0148	1.1984
9.00	122.40	0.7101	0.7101	0.1290	0.1290	0.0468	0.0468	0.0224	0.0224	0.0125	0.0125	0.0077	0.0048	0.0035	0.0026	0.0117	0.9511
12.25	166.60	0.5780	0.5780	0.1041	0.1041	0.0377	0.0377	0.0180	0.0180	0.0101	0.0100					0.0243	0.7721
16.00	217.60	0.4797	0.4797	0.0858	0.0858	0.0310	0.0310	0.0148	0.0148	0.0083	0.0083					0.0201	0.6397
20.25	275.40	0.4050	0.4050	0.0721	0.0721	0.0260	0.0260	0.0124	0.0124	0.0069	0.0069					0.0167	0.5391
25.00	340.00	0.3468	0.3468	0.0614	0.0614	0.0221	0.0221	0.0105	0.0105	0.0059	0.0059					0.0142	0.4609
36.00	489.60	0.2634	0.2634	0.0463	0.0463	0.0166	0.0166	0.0079	0.0079	0.0044	0.0044					0.0107	0.3493
49.00	666.40	0.2075	0.2075	0.0363	0.0363	0.0130	0.0130	0.0062	0.0062	0.0035	0.0034					0.0084	0.2748
72.25	989.40	0.1527	0.1526	0.0265	0.0265	0.0095	0.0095	0.0045	0.0045	0.0025	0.0025					0.0062	0.2018

a. See Ref. 4.
b. By interpolation.

Table II. Excitation cross sections among the sublevels of n = 2 → n' = 3 transition in units of πa_0^2. m is the absolute value of the magnetic quantum number. Cross sections in parabolic coordinates are designated by $Q(n_1\ n_2,\ n_1'\ n_2')$ with $n_1\, n_2$ and $n_1' n_2'$ belonging to the initial and the final states. Σ_1 is the sum of Q(2s) and Q(2p0), while Σ_2 is the sum of the three cross sections preceding Σ_2. Note has been taken of the relation $Q(n_1\ n_2,\ n_1'\ n_2') = Q(n_2\ n_1,\ n_2'\ n_1')$. The last two columns show the excitation cross section of n = 2 to n' = 3 in spherical and parabolic coordinates.

Impact Energy		m = 1		m = 0							Q(2,3)	
ryd	eV	Q(2p±1)[a]	2Q(00,01)	Q(2s)[b]	Q(2p0)[a]	Σ_1	2Q(01,02)	2Q(01,11)	2Q(01,20)	Σ_2	S	P
0.36	4.90	76.515	71.685	65.019	74.837	69.928	49.139	20.145	0.6227	69.907	73.222	70.796
0.64	8.70	57.440	57.441	49.441	64.529	56.985	39.983	16.628	0.3730	56.984	57.213	57.213
1.00	13.60	45.051	45.050	37.667	52.482	45.074	31.597	13.232	0.2448	45.074	45.063	45.062
1.44	19.58	35.937	35.938	29.488	42.803	36.146	25.323	10.649	0.1727	36.145	36.042	36.042
1.96	26.66	29.278	29.278	23.703	35.403	29.553	20.695	8.7283	0.1284	29.552	29.416	29.415
2.56	33.43	24.313	24.315	19.488	29.727	24.608	17.228	7.2813	0.0993	24.609	24.461	24.462
3.24	44.06	20.535	20.533	16.326	25.324	20.825	14.575	6.1694	0.0791	20.824	20.680	20.679
4.00	54.40	17.587	17.588	13.895	21.836	17.866	12.501	5.2987	0.0645	17.864	17.727	17.726
4.84	65.82	15.248	15.255	11.984	19.038	15.511	10.856	4.6066	0.0537	15.516	15.380	15.386
5.76	78.34	13.360	13.370	10.452	16.759	13.606	9.5244	4.0450	0.0454	13.615	13.483	13.493
6.76	91.94	11.812	11.813	9.206	14.876	12.041	8.4221	3.5795	0.0388	12.040	11.927	11.927
7.84	106.62	10.527	10.527	8.176	13.304	10.74	7.5112	3.1945	0.0336	10.739	10.634	10.633
9.00	122.40	9.447	9.448	7.317	11.976	9.647	6.7453	2.8704	0.0294	9.6451	9.547	9.547

a. See Ref. 6.
b. See Ref. 5.

Table III. Excitation cross sections of n = 2 level to n' = 4, 5, 6, 7, 8 levels in spherical and parabolic coordinates in units of πa_0^2. For spherical coordinates see Ref. 5,6.

Impact Energy		Q(2,4)		Q(2,5)		Q(2,6)		Q(2,7)		Q(2,8)		$\sum_{i=9}^{\infty} Q(2,i)$	Q(T)
ryd	eV	S	P	S	P	S	P	S	P	S[a]	P		
0.16	2.18												
0.2025	2.75		7.385										
0.25	3.40		12.016		3.933		1.706		0.868		0.491	0.570	92.037
0.36	4.90	13.362	13.227	4.977	4.941	2.459	2.435	1.392	1.395	0.879	0.880	1.566	95.240
0.64	8.70	10.791	10.794	4.117	4.104	2.059	2.049	1.182	1.186	0.752	0.753	1.351	77.433
1.00	13.60	8.335	8.334	3.168	3.151	1.575	1.570	0.907	0.907	0.576	0.576	1.033	60.633
1.44	19.58	6.539	6.538	2.467	2.456	1.226	1.220	0.704	0.704	0.444	0.446	0.800	48.206
1.96	26.66	5.251	5.250	1.970	1.960	0.972	0.971	0.560	0.559	0.357	0.354		
2.56	33.43	4.308	4.309	1.608	1.601	0.792	0.791	0.455	0.455	0.284	0.288		
3.24	44.06	3.602	3.602	1.338	1.332	0.656	0.657	0.378	0.378	0.238	0.239	0.427	27.314
4.00	54.40	3.059	3.059	1.132	1.127	0.556	0.555	0.319	0.319	0.202	0.201		
4.84	65.82	2.627	2.632	0.971	0.968	0.476	0.475	0.271	0.272	0.173	0.173		
5.76	78.34	2.292	2.293	0.843	0.840	0.413	0.412	0.237	0.236	0.149	0.149		
6.76	91.94	2.015	2.016	0.740	0.737	0.361	0.361	0.207	0.207	0.131	0.131		
7.84	106.62	1.787	1.792	0.653	0.652	0.319	0.319	0.183	0.183	0.116	0.116		
9.00	122.40	1.601	1.596	0.584	0.582	0.287	0.284	0.163	0.163	0.102	0.103		

a. By interpolation.

Table IV. Comparison of the excitation cross section for the transition n = 3 to n' = 4 in spherical and parabolic coordinates in units of πa_0^2. For spherical coordinates see Ref. 7.

Impact Energy	ryd	0.0543	0.0574	0.0616	0.0711	0.1988
	eV	0.7391	0.7809	0.8384	0.9675	2.704
Q(3,4)	S	400.66	481.35	555.96	653.24	617.59
	P	416.20	494.92	569.64	665.55	623.06
Impact Energy	ryd	0.2394	1.021	4.366	8.882	100.1
	eV	3.256	13.89	59.38	120.8	136.1
Q(3,4)	S	567.33	231.83	77.103	43.375	5.513
	P	572.67	233.86	77.884	44.088	6.704

Table V. Excitation cross section for the transition n = 3 to n' = 4, 5, 6, 7, 8, in units of πa_0^2.

Impact Energy		Q(3,4)	Q(3,5)	Q(3,6)	Q(3,7)	Q(3,8)	$\sum_{i=9}^{\infty}$ Q(3,i)	Q(T)
ryd	eV							
0.07	0.95	657.13						
0.08	1.09	709.21	83.365					
0.111	1.51	735.25	126.98	42.918	19.164	9.941	12.037	946.290
0.16	2.18	676.85	125.33	47.257	23.564	13.668	22.860	909.529
0.36	4.90	460.91	83.690	31.858	16.084	9.436	16.018	617.996
0.64	8.70	322.31	56.347	21.160	10.615	6.208	10.517	427.157
1.00	13.60	237.39	40.326	14.976	7.474	4.352	7.355	311.873
1.44	19.58	182.51	30.340	11.193	5.549	3.228		
1.96	26.66	145.08	23.692	8.689	4.290	2.489		
2.56	33.43	118.43	19.067	6.941	3.453	1.991		
3.24	44.06	98.510	15.709	5.699	2.805	1.621		
4.00	54.40	83.477	13.193	4.753	2.341	1.380	2.298	107.44
6.25	85.00	58.489	9.118	3.246	1.607	0.967		
9.00	122.4	43.624	6.713	2.377	1.186	0.661		

Table VI. Excitation cross section for the transition n = 4 to n' = 5, 6.

Impact Energy		Q(4,5)	Q(4,6)	$\sum_{i=7}^{\infty} Q(4,i)$	Q(T)
ryd	eV	πa_0^2	πa_0^2	πa_0^2	πa_0^2
0.03	0.408	3081.30			
0.04	0.544	3778.20	432.49		
0.0625	0.850	3794.63	660.11	548.98	5003.72
0.111	1.510	3137.40	570.52		
0.16	2.176	2583.94	462.07	474.59	3520.60
0.36	4.896	1566.94	264.25	269.03	2100.22
0.64	8.704	1049.78	169.66	171.37	1390.81
1.00	13.60	758.89	118.64	119.22	996.75
1.44	19.58	581.06	88.146		
1.96	26.66	450.49	68.524		
2.56	33.43	366.69	54.312		
3.24	44.06	306.32	44.569		
4.00	54.40	261.54	37.364		
6.25	85.00	190.23	25.869		
9.00	122.4	150.46	19.385		

Table VII. Excitation cross section for the transition n = 5 to n' = 6 in units of πa_0^2.

Impact Energy	ryd	0.0169	0.0225	0.04	0.111	0.16
	eV	0.230	0.306	0.544	1.510	2.176
Q(5,6)	πa_0^2	11,307.87	13,791.58	13,588.04	8,698.01	6,889.87
Impact Energy	ryd	0.36	0.64	1.00	1.44	1.96
	eV	4.896	8.704	13.60	19.58	26.66
Q(5,6)	πa_0^2	3,979.62	2,628.03	1,907.17	1,485.27	1,221.40
Impact Energy	ryd	2.56	3.24	4.00	6.25	9.00
	eV	33.43	44.06	54.40	85.00	122.4
Q(5,6)	πa_0^2	1,047.77	928.78	844.50	718.80	654.35

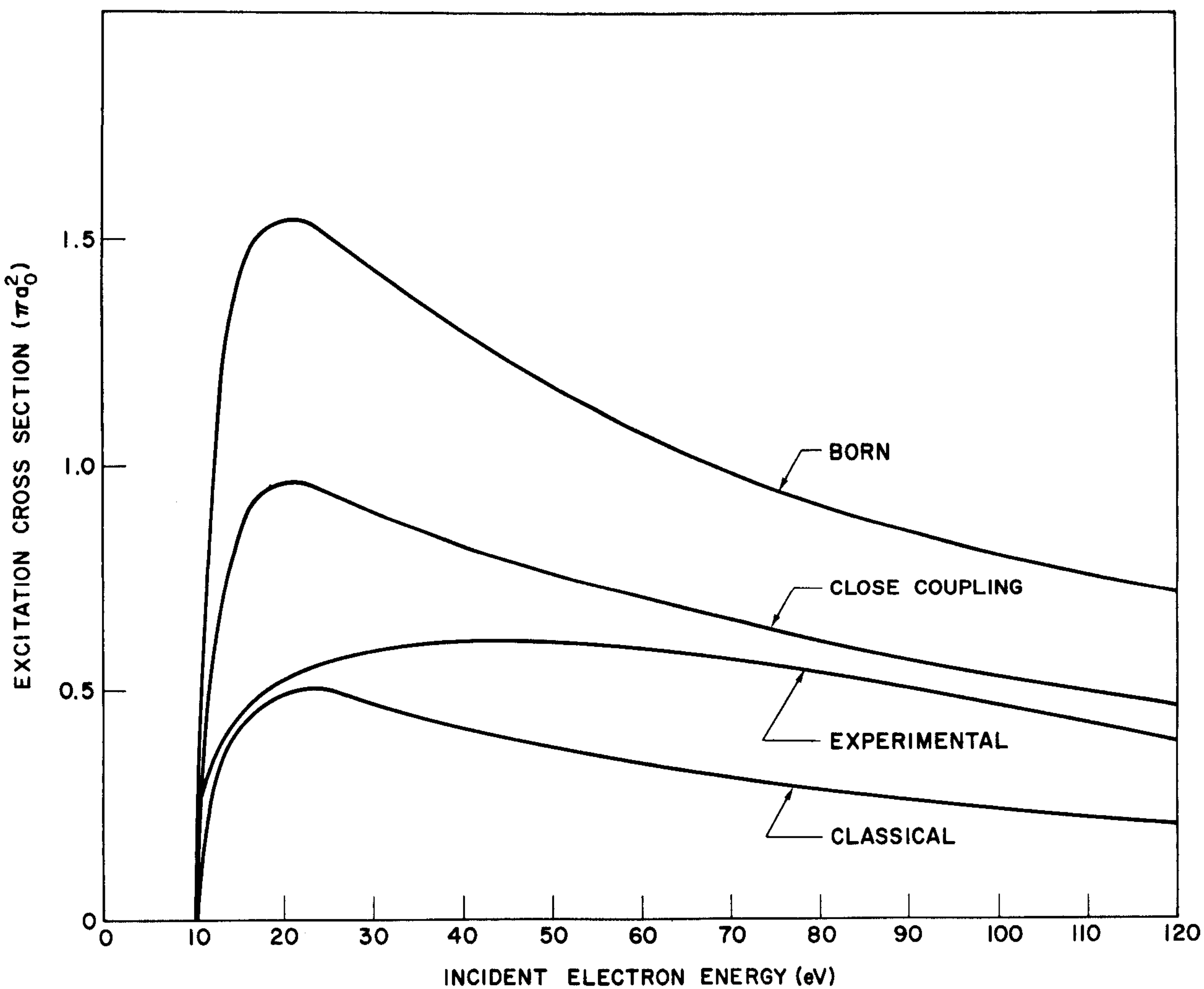

Fig. 1. Excitation of the ground state of the hydrogen atom to the n = 2 states by electron collision. The theoretical curves, Born, close coupling and classical, are compared with the experimental curve.

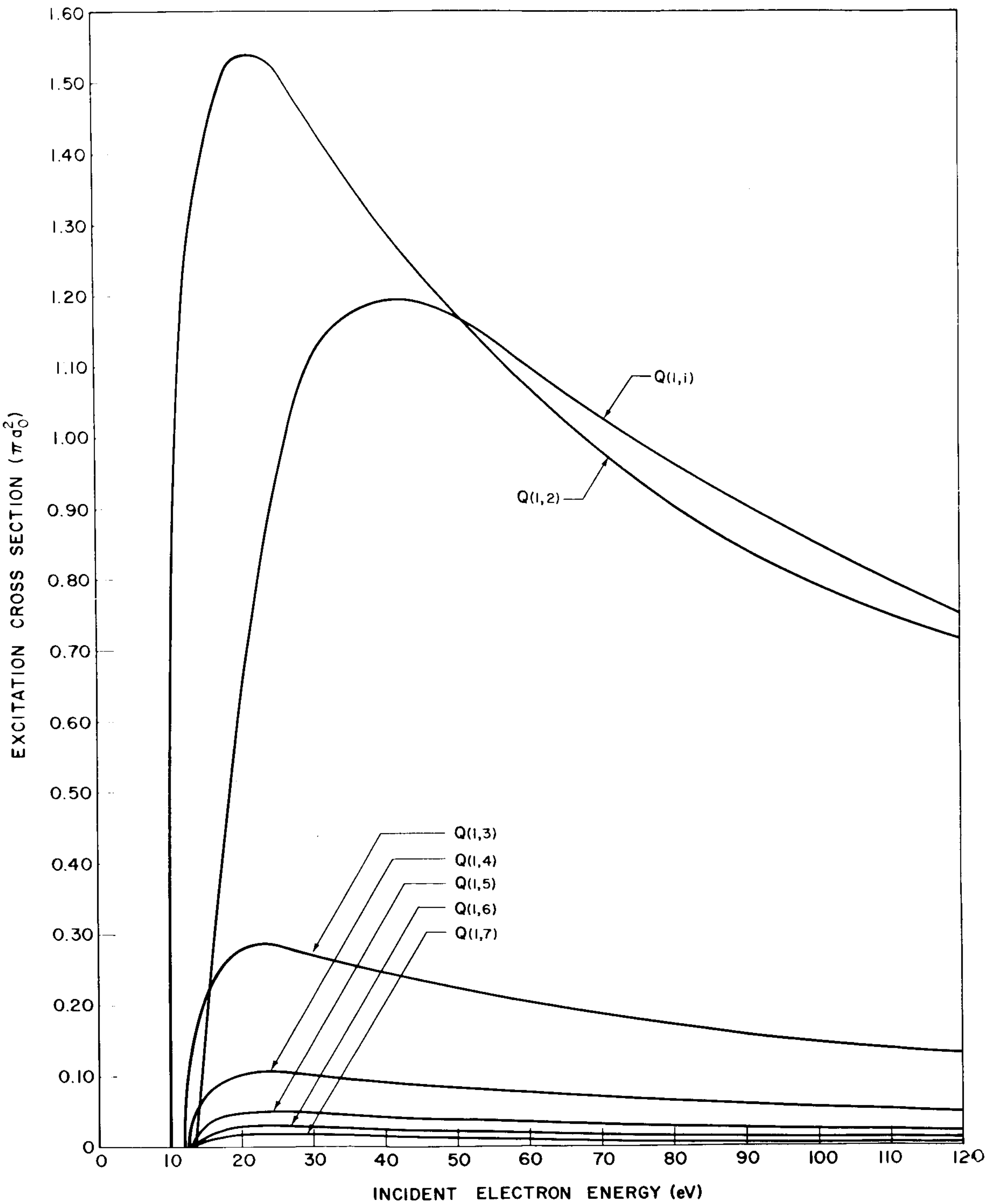

Fig. 2. Excitation of the ground state of the hydrogen to the n = 2, 3, 4, 5, 6, 7 states. Q(1,i) is the ionization cross section of the ground state by electron collision.

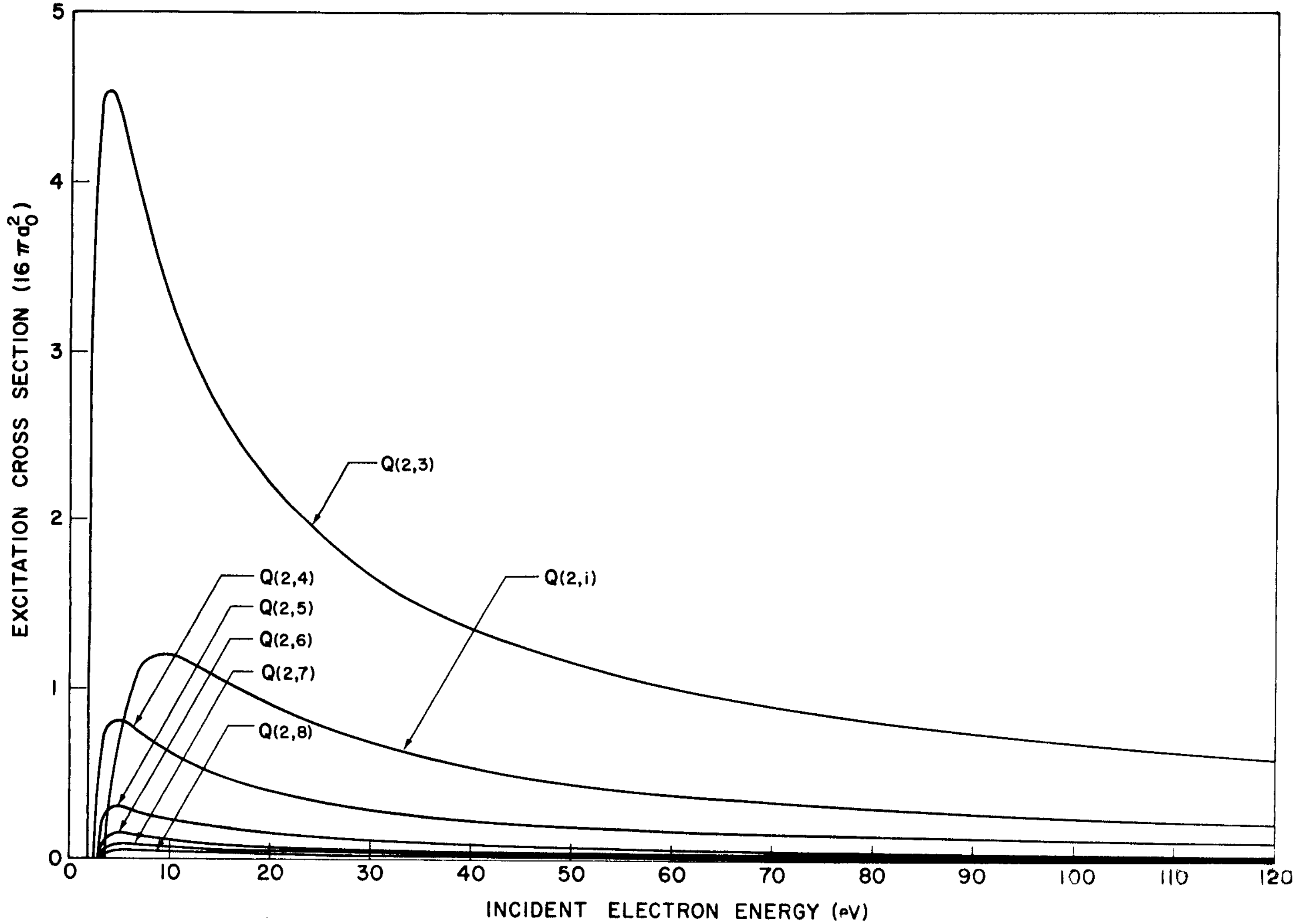

Fig. 3. Excitation of the n = 2 states to the n = 3, 4, 5, 6, 7, 8 states. Q(2,i) is the ionization cross section of the n = 2 states.

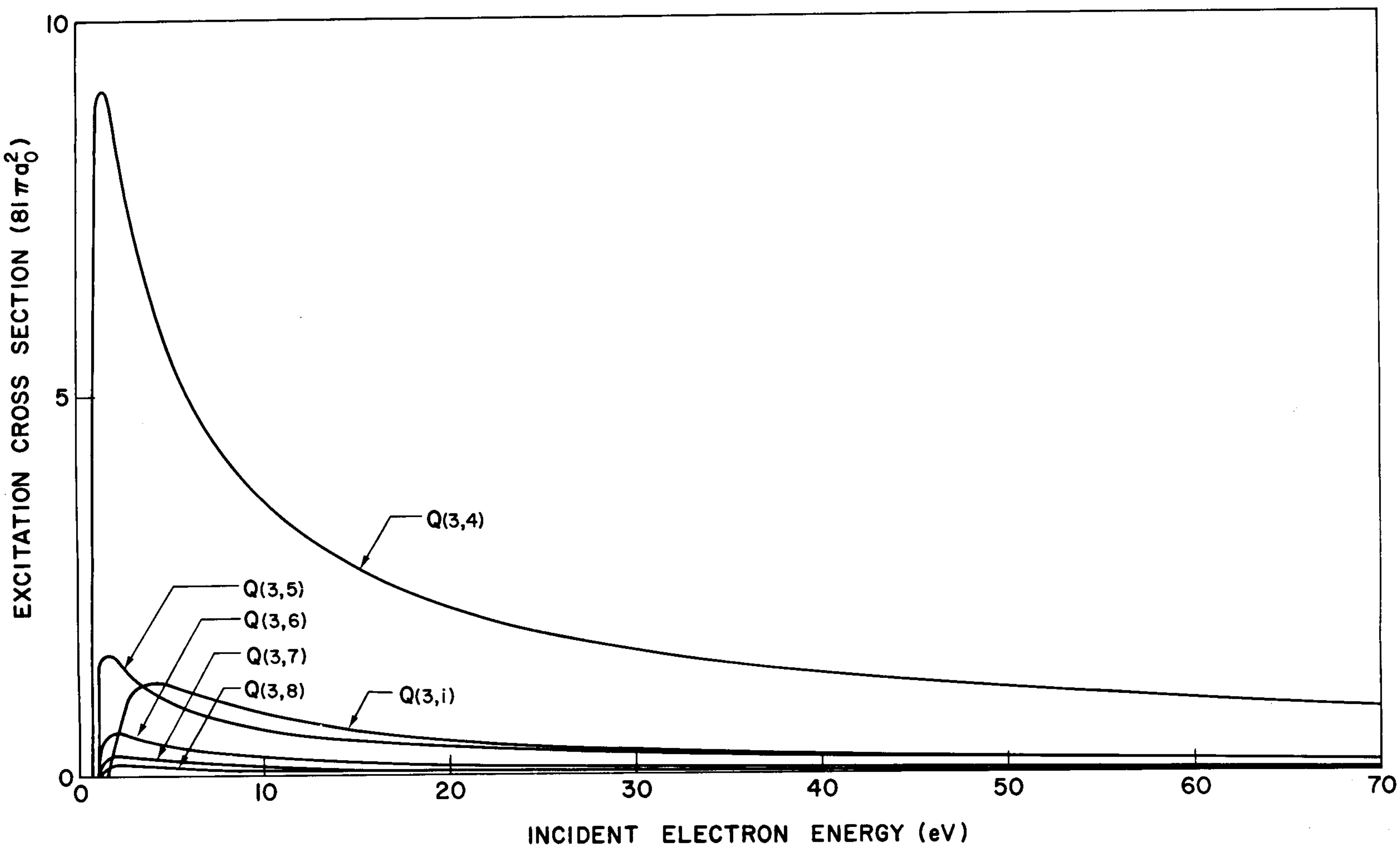

Fig. 4. Excitation of the n = 3 states to the n = 4, 5, 6, 7, 8 states. Q(3,i) is the ionization cross section of the n = 3 states.

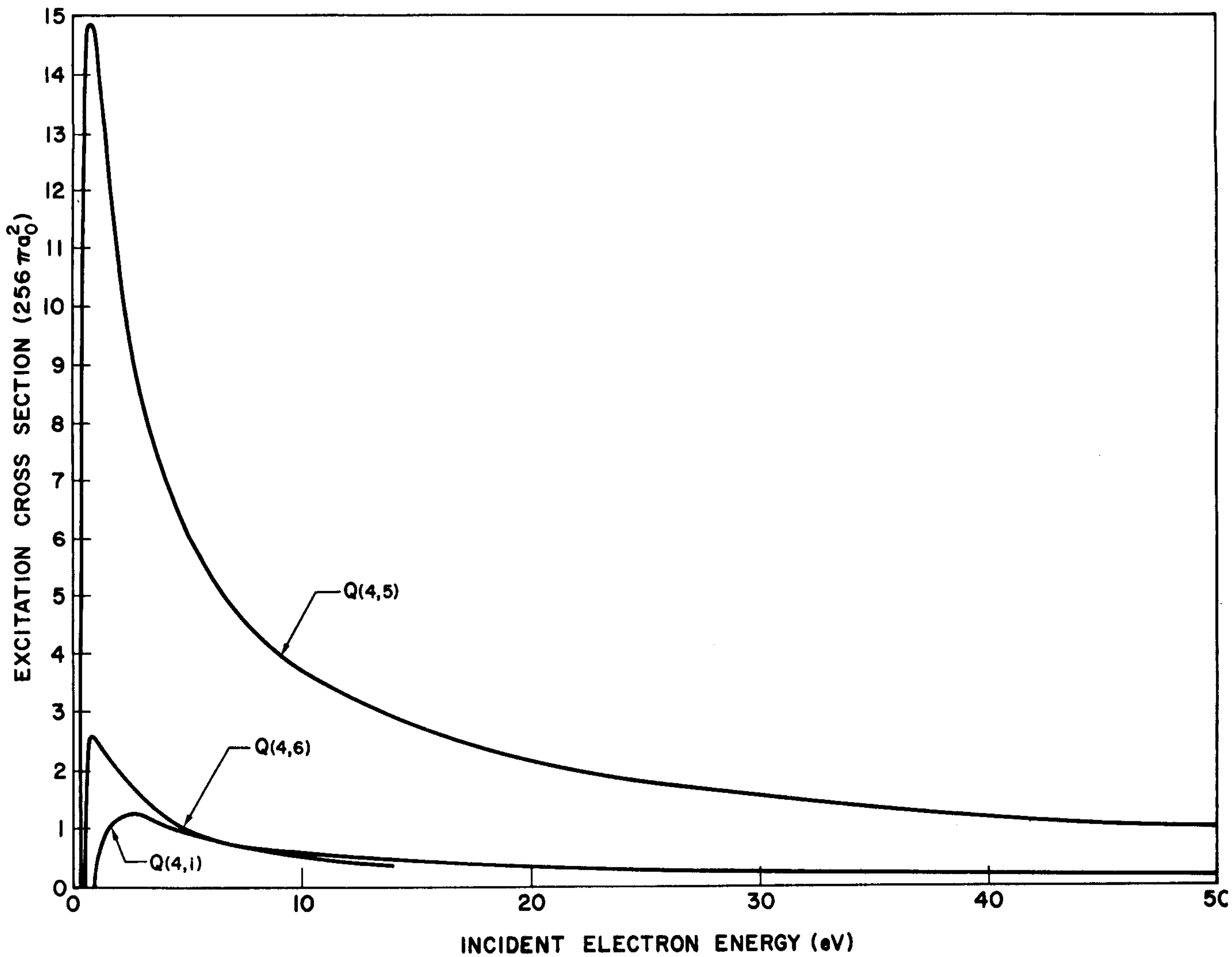

Fig. 5. Excitation of the n = 4 states to the n = 5, 6 states. Q(4, i) is the ionization cross section of the n = 4 states.

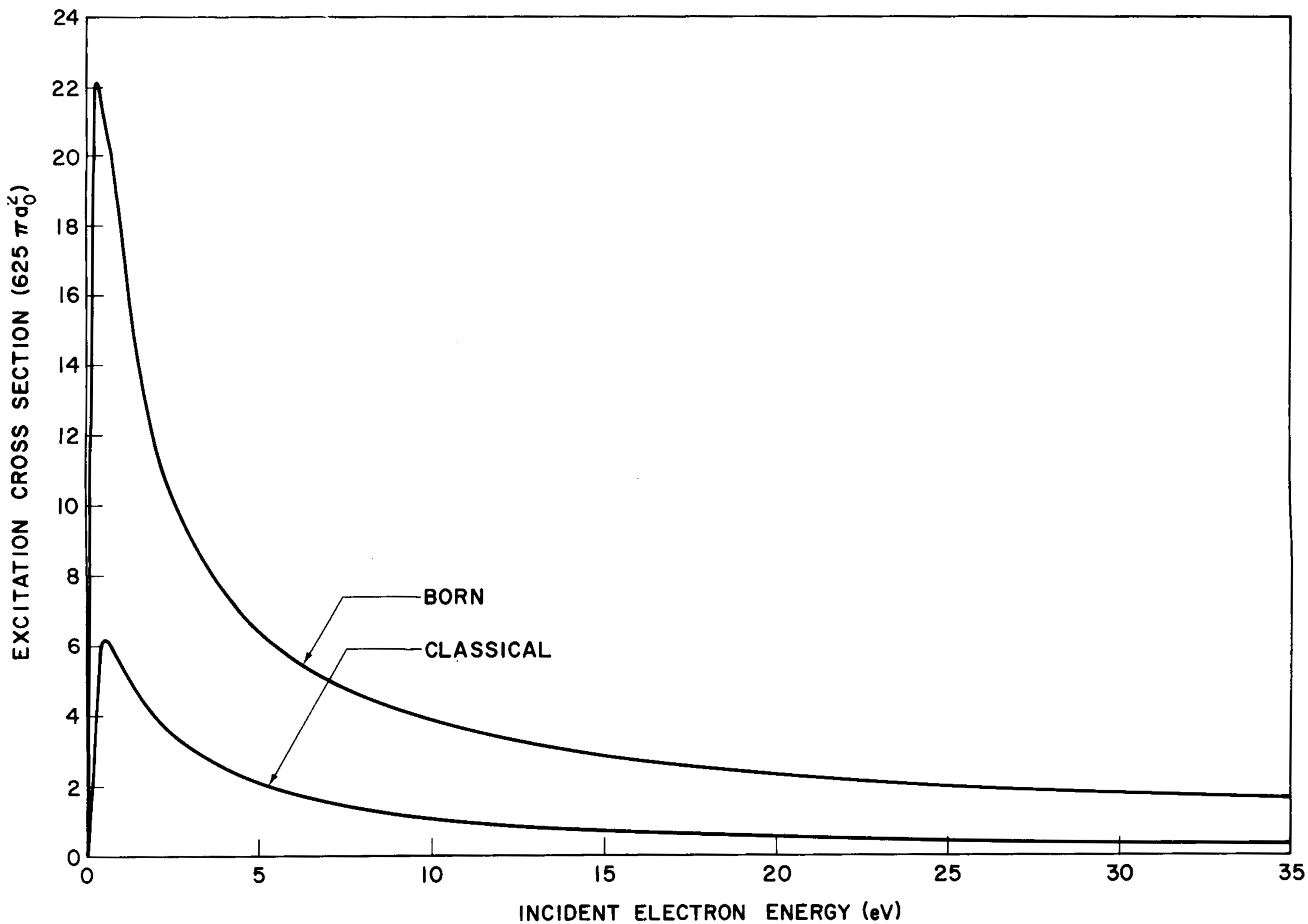

Fig. 6. Excitation of the n = 5 states to the n = 6 states. The classical curve is compared with the Born approximation curve.

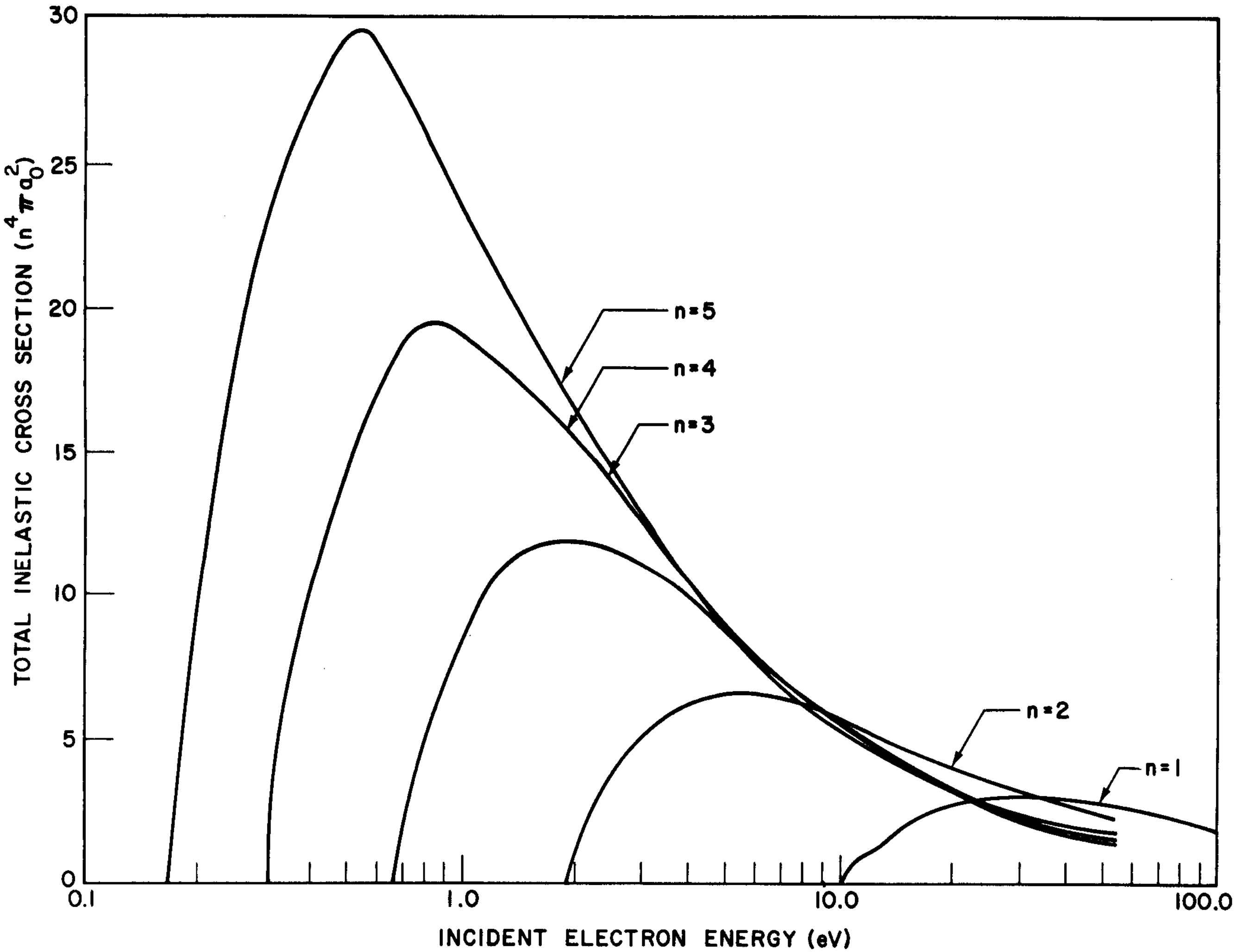

Fig. 7. Total inelastic, including excitation to all states and ionization, cross section of the hydrogen atom by electron collision. Different curves correspond to the atom initially in any of the states n = 1, 2, 3, 4, and 5.